

Composite Boson Mapping for Lattice Boson Systems

Daniel Hueriga,¹ Jorge Dukelsky,¹ and Gustavo E. Scuseria²

¹*Instituto de Estructura de la Materia, C.S.I.C., Serrano 123, E-28006 Madrid, Spain*

²*Department of Chemistry and Department of Physics and Astronomy, Rice University, Houston, TX 77005, USA*

We present a canonical mapping transforming physical boson operators into quadratic products of cluster composite bosons that preserves matrix elements of operators when a physical constraint is enforced. We map the 2D lattice Bose-Hubbard Hamiltonian into 2×2 composite bosons and solve it at mean field. The resulting Mott insulator-superfluid phase diagram reproduces well Quantum Monte Carlo results. The Higgs boson behavior along the particle-hole symmetry line is unraveled and in remarkable agreement with experiment. Results for the properties of the ground and excited states are competitive with other state-of-the-art approaches, but at a fraction of their computational cost. The composite boson mapping here introduced can be readily applied to frustrated many-body systems where most methodologies face significant hurdles.

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Introduction.— In the past few years, there has been great experimental progress on the control and manipulation of cold atomic gases loaded in optical lattices, leading to quantum simulators of the Bose-Hubbard model and its Mott insulator to superfluid transition [1]. A notable recent experiment has revealed the Higgs boson behavior across this transition in a 2D optical lattice [2]. There is currently great interest in cold atomic physics for engineering synthetic gauge fields that induce topological phases and phase transitions. This can be accomplished using a combination of laser-induced tunneling with superlattice techniques [3], or by time-periodic shaking of the lattice [4]. From the theoretical perspective, traditional mean field approaches can describe the phase diagram of bosonic atoms in lattices of various geometries, but only qualitatively [5, 6]. Quantum Monte Carlo (QMC) yields a highly accurate description of ground state properties at zero and finite temperatures whenever the system has no frustration [7, 8]. Static and dynamic properties have also been studied with the Variational Cluster Approximation (VCA) [9, 10]. Extensions of static mean field approaches involving the use of clusters have been considered [11–13]. In this work, we introduce a theory that maps cluster subspaces of the original Fock space onto composite bosons containing the *exact* internal dynamics of the cluster, and whose interactions account for residual correlations between the clusters. Because the mapping is canonical, it is then possible to apply standard many-body techniques to this Composite Boson (CB) Hamiltonian. In this sense, the present model builds upon Hierarchical Mean Field Theory (HMFT) for quantum magnetism [14]. These ideas are here extended to interacting bosons systems loaded in optical lattices. We refer to the resulting model as Composite Boson Mean Field Theory (CBMFT). We demonstrate that the inclusion of higher order fluctuation terms in the composite mean field yields very accurate results. The CB approach to the Bose-Hubbard model unravels the Higgs boson behavior along the particle-hole sym-

metry line and yields remarkable agreement with experimental data [2].

Composite Boson Mapping.— Let us start our derivation by assuming a quadratic mapping of the elementary boson creation (annihilation) operators a_i^\dagger (a_i) at site i in terms of a generic set of CB b_α^\dagger (b_α).

$$a_i^\dagger = \sum_{\alpha\beta} U_{i\alpha\beta}^* b_\alpha^\dagger b_\beta, \quad a_i = \sum_{\alpha\beta} U_{i\alpha\beta} b_\alpha^\dagger b_\beta. \quad (1)$$

If the states $|\alpha\rangle$ of the CB space are known, the matrix U is formally defined as $U_{i\alpha\beta}^* = \langle\alpha| a_i^\dagger |\beta\rangle$ and $U_{i\beta\alpha} = \langle\alpha| a_i |\beta\rangle$, and has *unitary* character in the Wigner definition. Let us now explore the conditions which should be fulfilled by transformation (1) in order to preserve the canonical bosonic commutation relations $[a_i, a_j^\dagger] = \delta_{i,j}$. Inserting the transformation in the commutator we obtain

$$[a_i, a_j^\dagger] = \sum_{\alpha\beta\beta'} (U_{i\alpha\beta} U_{j\alpha\beta'}^* - U_{i\beta'\alpha} U_{j\beta\alpha}^*) b_\beta^\dagger b_{\beta'} = \sum_{\alpha\beta\beta'} \left(\langle\beta| a_i |\alpha\rangle \langle\alpha| a_j^\dagger |\beta'\rangle - \langle\beta| a_j^\dagger |\alpha\rangle \langle\alpha| a_i |\beta'\rangle \right) b_\beta^\dagger b_{\beta'}.$$

The satisfaction of the canonical commutation relations rely on *i*) resolution of the identity, $\sum_\alpha |\alpha\rangle \langle\alpha| = I$, and *ii*) fulfillment of the physical constraint, $\sum_\alpha b_\alpha^\dagger b_\alpha = I$. Both conditions are equivalent and can be satisfied by choosing a complete set of states of the composite Hilbert space. However, the mapping has no significant power at this stage, as we would still have to deal with the whole Fock space of the system. Therefore, we divide it into clusters and derive an exact Hamiltonian by means of the corresponding *cluster composite bosons*. Following this idea, any operator that is an algebraic function of the original operators a_i within a single cluster will be mapped to a one-body operator of the CB space. In the same way, any product of operators belonging to N different clusters will be mapped to an N -body operator.

Therefore, a general two-body boson Hamiltonian would lead to a four-body CB interaction. For the sake of simplicity, we will here restrict ourselves to a density-density interaction that leads to a two-body CB Hamiltonian, since each density operator is contained in a single cluster. Let us assume a general Hamiltonian of this kind

$$H = \sum_{ij} \left[t_{ij} a_i^\dagger a_j + V_{ij} n_i n_j \right], \quad n_i = a_i^\dagger a_i. \quad (3)$$

We start our derivation assuming a square lattice partitioned into a set of M clusters, each one at position R of a CB superlattice and containing $L \times L$ sites. We assume a perfect tiling between the superlattice of CB bosons and the original lattice. Next, we formally map the Hamiltonian using the prescription described above and rewrite it in terms of CB labeled by the occupation configuration of each cluster, $\mathbf{n} \equiv \{n_1, \dots, n_L, \dots, n_{L^2}\}$,

$$H_{CB} = \sum_{R\mathbf{n}\mathbf{m}} \langle R\mathbf{n} | H | R\mathbf{m} \rangle b_{R\mathbf{n}}^\dagger b_{R\mathbf{m}} + \sum_{RR'} \sum_{\mathbf{n}\mathbf{n}'\mathbf{m}\mathbf{m}'} \langle R\mathbf{n}R'\mathbf{n}' | H | R\mathbf{m}R'\mathbf{m}' \rangle \times b_{R\mathbf{n}}^\dagger b_{R'\mathbf{n}'}^\dagger b_{R\mathbf{m}} b_{R'\mathbf{m}'}. \quad (4)$$

For reasons that will become clear below, we will perform a generic unitary transformation among the CBs, $b_{R\alpha}^\dagger = \sum_{\mathbf{n}} U_{R\mathbf{n}}^\alpha b_{R\mathbf{n}}^\dagger$. In this particular case, we are interested in a uniform and real ground-state wavefunction, therefore, we will drop the superlattice site index R from now on. In this new basis, the hamiltonian can be written as

$$H_{CB} = \sum_R \sum_{\alpha\beta} T_{\beta}^\alpha b_{R\alpha}^\dagger b_{R\beta} + \sum_{RR'} \sum_{\alpha\alpha'\beta\beta'} W_{\beta\beta'}^{\alpha\alpha'} b_{R\alpha}^\dagger b_{R'\alpha'}^\dagger b_{R\beta} b_{R'\beta'}, \quad (5)$$

where the matrix elements

$$T_{\beta}^\alpha = \sum_{\mathbf{n}, \mathbf{m}} \langle \mathbf{n} | H | \mathbf{m} \rangle U_{\mathbf{n}}^\alpha U_{\mathbf{m}}^\beta \quad (6)$$

$$W_{\beta\beta'}^{\alpha\alpha'} = \sum_{\mathbf{n}\mathbf{n}'\mathbf{m}\mathbf{m}'} \langle \mathbf{n}\mathbf{n}' | H | \mathbf{m}\mathbf{m}' \rangle U_{\mathbf{n}}^\alpha U_{\mathbf{n}'}^{\alpha'} U_{\mathbf{m}}^\beta U_{\mathbf{m}'}^{\beta'} \quad (7)$$

encode all the information of the original Hamiltonian. Notice that, in general, $\langle \mathbf{n}\mathbf{n}' | H | \mathbf{m}\mathbf{m}' \rangle$ depends on the precise layout of the two considered neighboring clusters. The CB Hamiltonian (5) is an exact image of the original boson Hamiltonian provided that the physical constraint in each cluster site ($\sum_{\alpha} b_{R\alpha}^\dagger b_{R\alpha} = I$) is satisfied. On the other hand, treating this Hamiltonian by means of standard many-body techniques, we immediately incorporate quantum correlations inside the cluster in an exact way.

Composite Boson Mean Field Theory.— We here treat the CB Hamiltonian in the Bogoliubov-de Gennes approximation. In order to proceed further, we have to

specify the matrix elements of the initial lattice Hamiltonian. As a first test of CBMFT, we benchmark the Bose-Hubbard Hamiltonian in a 2D square lattice. Namely, $t_{ij} = -t\delta_{i,j+\mathbf{e}}$ where \mathbf{e} is the unit vector in the lattice directions \mathbf{x} , \mathbf{y} , and $V_{ij} = U\delta_{i,j}$ is the on-site Hubbard repulsion. In what follows, we omit U and measure all quantities in units of U . Assuming a uniform 2D lattice with translational symmetry, we first perform a Fourier transform of the CB boson operators $b_{R\alpha}^\dagger = (1/\sqrt{M}) \sum_{\mathbf{k}} e^{-iL\mathbf{k}\cdot\mathbf{R}} b_{\mathbf{k}\alpha}^\dagger$, leading to

$$H_{CB} = \sum_{\alpha\beta} T_{\beta}^\alpha \sum_{\mathbf{k}} b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\beta} + \frac{1}{M} \sum_{\alpha\alpha'\beta\beta'} W_{\beta\beta'}^{\alpha\alpha'} \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{q}} \gamma_{\mathbf{q}} b_{\mathbf{k}_1\alpha}^\dagger b_{\mathbf{k}_2+\mathbf{q}\alpha'}^\dagger b_{\mathbf{k}_1+\mathbf{q}\beta} b_{\mathbf{k}_2\beta'}, \quad (8)$$

where we have introduced $\gamma_{\mathbf{q}} = \cos(Lq_x) + \cos(Lq_y)$ after a symmetrization of the two-body matrix elements $W_{\beta\beta'}^{\alpha\alpha'}$ in order to preserve the lattice C_4 symmetry. Details on the calculation of these matrix elements can be found in the Supplemental Material. Next, we assume a condensation of the CB in the $\mathbf{k} = \mathbf{0}, \alpha = 0$ state by introducing a shift transformation $b_{\mathbf{k}=\mathbf{0},\alpha=0} = b_{\mathbf{k}=\mathbf{0},\alpha=0}^\dagger = \sigma\sqrt{M}$. This transformation manifestly violates the on-site physical constraint. Thus, we relax it and impose a global constraint on the CB density, $\sum_R \sum_{\alpha} b_{R\alpha}^\dagger b_{R\alpha} = M$. Transforming to momentum space and shifting, the global physical constraint becomes

$$\sigma^2 + \frac{1}{M} \sum_{\alpha \neq 0} \sum_{\mathbf{k}} b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha} = 1 \quad (9)$$

where we have neglected the fluctuations of the condensed boson. Eq. (9) defines σ^2 as the CB condensate fraction. Inserting the constraint (9) by means of a Lagrange multiplier λ in the CB Hamiltonian (8) and applying a mean field decoupling, we arrive to a quadratic Hamiltonian of the form

$$H_{MF} = H^{(0)} + \sum_{\mathbf{k}\alpha\beta} A_{\mathbf{k}\alpha\beta} b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\beta} + \sum_{\mathbf{k}\alpha\beta} \left(B_{\mathbf{k}\alpha\beta} b_{\mathbf{k}\alpha}^\dagger b_{-\mathbf{k}\beta}^\dagger + B_{\mathbf{k}\alpha\beta} b_{-\mathbf{k}\beta} b_{\mathbf{k}\alpha} \right) \quad (10)$$

where the specific form of $H^{(0)}$ and the matrices $A_{\mathbf{k}\alpha\beta}$ and $B_{\mathbf{k}\alpha\beta}$ can be found in the Supplemental Material.

The quadratic mean field Hamiltonian (10) can be diagonalized by means of a Bogoliubov transformation $c_{\mathbf{k}\alpha}^\dagger = \sum_{\beta} X_{\mathbf{k}\beta\alpha} b_{\mathbf{k}\beta}^\dagger - \sum_{\beta} Y_{\mathbf{k}\alpha\beta} b_{-\mathbf{k}\beta}$, leading to the Bogoliubov eigenvalue equation [15]

$$\begin{pmatrix} A_{\mathbf{k}} & 2B_{\mathbf{k}} \\ -2B_{\mathbf{k}}^* & -A_{\mathbf{k}}^* \end{pmatrix} \begin{pmatrix} X_{\mathbf{k}} \\ Y_{\mathbf{k}} \end{pmatrix} = \omega_{\mathbf{k}} \begin{pmatrix} X_{\mathbf{k}} \\ Y_{\mathbf{k}} \end{pmatrix}, \quad (11)$$

where the positive eigenvalues $\omega_{\mathbf{k}}$ determine the excitation spectrum. The Bogoliubov equation depends on the

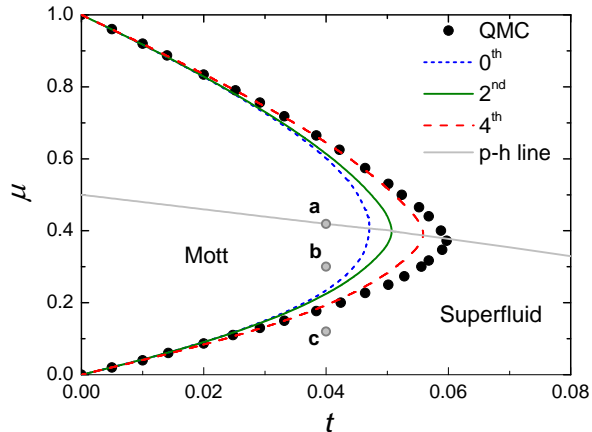


FIG. 1: (color online) Phase diagram of the first lobe of the Mott-insulator to superfluid transition. The dotted, solid, and dashed curves show the composite 2×2 boson mean field results in increasing order of approximation. The particle-hole symmetry line traverses the Mott and superfluid regions. Black circles are QMC results from Ref. [7]. Grey circles display three points in parameter space for which the dispersions are analyzed in Fig. 3.

generic transformation U previously defined. We are now ready to derive a Hartree-Bose (HB) like equation for this transformation upon minimization of the free energy with respect to the condensed CB structure $U_{\mathbf{m}}^0$. The resulting equation can be cast in matrix form

$$\sum_{\mathbf{n}} h_{\mathbf{m},\mathbf{n}} U_{\mathbf{n}}^0 = \lambda U_{\mathbf{m}}^0. \quad (12)$$

The derivation of the matrix elements of h for $L \times L$ clusters, given in the Supplemental Material, is straightforward though lengthy. The HB Hamiltonian h depends on the Hartree transformation U , on the Bogoliubov amplitudes $X_{\mathbf{k}}$, $Y_{\mathbf{k}}$, and on the fraction of the condensate σ^2 . Strictly speaking, the self-consistent Hartree diagonalization provides a single eigenvector defining the structure of the condensed CB and the corresponding lowest eigenvalue, which is the Lagrange multiplier λ . However, after attaining self-consistency the matrix diagonalization procedure supplies a complete set of eigenstates that are orthogonal to the condensed CB. It is in this basis orthogonal to the condensate where the Bogoliubov Hamiltonian (10) is expressed. We seek a self-consistent solution of the coupled set of equations determined by the diagonalization of the HB Hamiltonian (12) that fixes the Hartree transformation U and the Lagrange multiplier λ , and the Bogoliubov equations (11) that provides the Bogoliubov amplitudes $X_{\mathbf{k}}$ and $Y_{\mathbf{k}}$, together with the expectation value of the physical condition (9) for the determination of the CB condensed fraction σ^2 .

2D Bose-Hubbard Model Results.— We start with benchmark calculations describing the insulating Mott phase in the first lobe corresponding to a density per site of $\rho = 1$ and cluster size of 2×2 . Within this phase, the structure of the Hartree transformation U and the CB condensed fraction σ^2 are μ -independent. The structure of the condensed CB dictated by U^0 is a linear combination of cluster states with $N = 4$ physical bosons. The CB fluctuations are pairs of *particle* ($N = 5$) and *hole* ($N = 3$) physical bosonic states. In addition, particle- and hole-like excitation eigenvalues have a linear dependence on the chemical potential for fixed t . Both excitations cross each other at the *particle-hole symmetry line*, where the gap is doubly degenerate. The edges of the first Mott lobe are determined by the vanishing of the gap, indicating the appearance of a Goldstone mode at $\mathbf{k} = \mathbf{0}$ related to the $U(1)$ symmetry breaking in the superfluid. Fig. 1 shows the phase diagram of the Bose-Hubbard model in three different CB mean field approximations. The 0^{th} order approximation neglects fluctuations and solves the Hartree equations exclusively. The edges of the Mott lobe are determined in this case by a deviation from the density $\rho = 1$. This 0^{th} order approximation is equivalent to the cluster mean field calculations of Refs. [11–13]. The 2^{nd} and 4^{th} order approximations incorporate fluctuations by means of a self-consistent solution of the Bogoliubov (11) plus Hartree (12) equations linked by the physical condition (9). The 2^{nd} order approximation neglects two-body interactions between fluctuating bosons, while the 4^{th} order solves the three coupled equations in full. As the approximation order increases, CBMFT shows clear convergence towards QMC. Also shown in Fig. 1 is the extension of the particle-hole line to the superfluid phase characterized by density $\rho = 1$.

The full self-consistent 4^{th} order approximation does not describe the gapless feature of the superfluid phase correctly. Although ways to correct this deficiency have been suggested [16], in the rest of this paper we will focus on the 2^{nd} order approximation that strictly preserves the gapless spectrum when $U(1)$ symmetry is broken.

Fig. 2 shows the total density $\rho = \langle \phi | a_j^\dagger a_j | \phi \rangle$ and the condensate density $\rho_c = |\langle \phi | a_j^\dagger | \phi \rangle|^2$ for hopping values of $t = 0.02$ and 0.04 . VCA results for $t = 0.02$ [9, 10] compare well with our results in Fig. 2. The plateau characterizing the Mott phase is reduced for larger t . Outside this region, the superfluid has non-commensurate density in the entire phase diagram except for the particle-hole (p-h) line. The condensate density of physical bosons, representing the coherence of the superfluid phase, vanishes in the Mott phase.

In Fig. 1, we have depicted three characteristic points at $t = 0.04$; namely, **a** is at the p-h line in the Mott phase, **b** is still in the Mott phase but away from the p-h line, and **c** is in the superfluid phase. Fig. 3 shows particle- and hole-like excitations for $k_y = 0$ as a function of k_x for

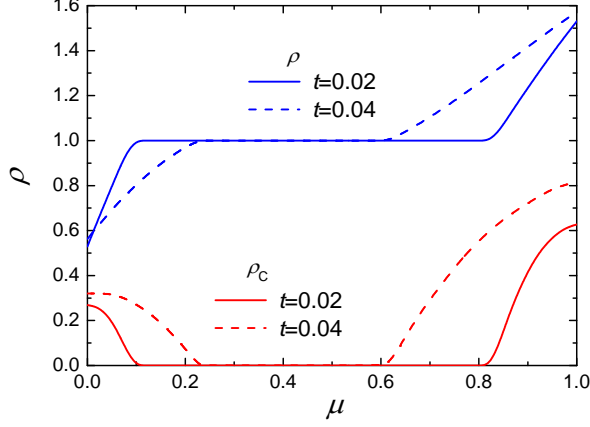


FIG. 2: (color online). Total density (ρ) and condensate density (ρ_c) for $t = 0.02$ (solid line) and $t = 0.04$ (dashed line) within the second order approximation.

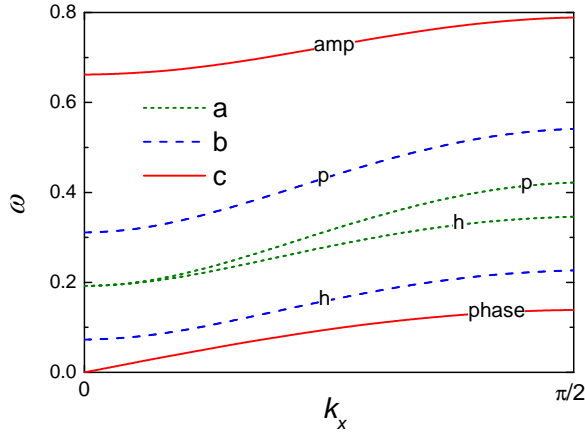


FIG. 3: (color online). Dispersion modes for $t = 0.04$: particle- and hole-like excitation modes at (a) the particle-hole symmetry line ($\mu = 0.419$), and (b) inside the Mott insulator ($\mu = 0.30$), and amplitude- and phase-like modes at (c) in the superfluid ($\mu = 0.12$).

a and **b** inside the Mott phase. The degeneracy of the particle and hole modes for point **a** approaching $\mathbf{k} = \mathbf{0}$ is clearly seen in this figure. Away from the p-h line and still in the Mott phase (point **b**), this degeneracy is broken and the hole is favored against the particle mode. Well inside the superfluid phase (point **c**), we recognize a gapless mode (Goldstone) with the characteristic linear dispersion at low momentum, as well as a gapped mode. An analysis of the CB structure $U_{\mathbf{m}}^{\alpha}$ of each mode, similar to the one performed in Ref. [11] shows that the gapless mode is a phase-like mode, while the gapped mode is an amplitude-like mode.

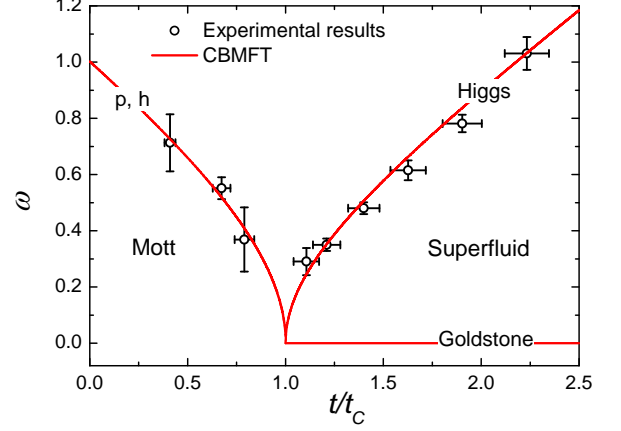


FIG. 4: (color online). Higgs, Goldstone, particle, and hole modes along the p-h symmetry line computed within 2^{nd} order CBMFT (solid line). Experimental data points from [2].

As already shown in Fig. 1, the p-h line crosses the tip of the Mott lobe where the quantum phase transition is driven at constant density ($\rho = 1$). The phase transition at the lobe tip can be understood within the Higgs mechanism, as has been recently discussed in Refs. [2, 17]. Fig. 4 displays how doubly degenerate excitations along the p-h line inside the Mott insulator vanish at the critical point. In the superfluid region, one of them remains at zero excitation energy (Goldstone) while the other one grows for increasing hopping (Higgs). In both cases, their structure mixes particle- and hole-like states of the cluster. The CBMFT results not only match the experimental data [2] remarkably well but also gives an excellent description of the critical point.

Conclusions.— We have introduced a cluster composite boson mapping which separates intra- and inter-cluster degrees of freedom. The former are treated exactly while the latter can be approximated using standard many-body methods applied to the resulting CB Hamiltonian. We have here shown that a mean field approximation to the CB interaction for the Bose-Hubbard model produces an accurate description of the Mott-superfluid phase diagram compared to QMC results. Densities and dispersions are found in quantitative agreement with more sophisticated techniques like VCA. The recently measured Higgs mode is also computed and found to be in remarkable agreement with experiment. Further improvement of the theory beyond the mean field second-order approximation employed in this paper is feasible. Most importantly, CBMFT is readily applicable to other many-body problems where frustration, synthetic gauge fields or long range interactions pose significant hurdles to existing state-of-the-art methodologies.

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SUPPLEMENTAL MATERIAL

Matrix Elements of the CB Hamiltonian

The cluster-cluster interaction matrix elements depend on the particular layout of the two clusters R and R' . For the Bose-Hubbard model, it is exclusively related to the hopping term that destroys (creates) a boson at the edge of one cluster and creates (destroys) a boson at the edge of a neighbor cluster. The specific form of the interaction for $L \times L$ clusters is

$$W_{\beta\beta'}^{\alpha\alpha'}(R, R') = \sum_{\langle i,j \rangle} \sum_{\mathbf{n}, \mathbf{n}'} \left(\sqrt{n_i+1} \sqrt{n'_j} U_{R\{n_i+1\}}^{\alpha} U_{R'\{n'_j-1\}}^{\alpha'} U_{R\mathbf{n}}^{\beta} U_{R'\mathbf{n}'}^{\beta'} + \sqrt{n_i} \sqrt{n'_j+1} U_{R\{n_i-1\}}^{\alpha} U_{R'\{n'_j+1\}}^{\alpha'} U_{R\mathbf{n}}^{\beta} U_{R'\mathbf{n}'}^{\beta'} \right), \quad (13)$$

where $\sum_{\langle i,j \rangle}$ runs over the L links between the edges of both clusters with $i \in R$ and $j \in R'$. Using compact notation, $\{n_i+1\}$ corresponds to a configuration \mathbf{n} with one more boson at site i , that is, $\{n_i+1\} \equiv (n_1, \dots, n_i+1, \dots, n_{L^2})$.

Next, we perform the C_4 symmetrization of the matrix elements (13) in order to preserve the lattice symmetry at the mean field level

$$W_{\beta\beta'}^{\alpha\alpha'} = \frac{1}{4} \sum_{\langle i,j \rangle} \sum_{\mathbf{n}, \mathbf{n}'} \left(\sqrt{n_i+1} \sqrt{n'_j} U_{\{n_i+1\}}^{\alpha} U_{\{n'_j-1\}}^{\alpha'} U_{\mathbf{n}}^{\beta} U_{\mathbf{n}'}^{\beta'} + \sqrt{n_i} \sqrt{n'_j+1} U_{\{n_i-1\}}^{\alpha} U_{\{n'_j+1\}}^{\alpha'} U_{\mathbf{n}}^{\beta} U_{\mathbf{n}'}^{\beta'} \right), \quad (14)$$

where now $\sum_{\langle i,j \rangle}$ runs over the $L \times L$ links which connects cluster R with the four nearest neighbors R' . The intra-cluster one-body matrix elements has both contributions, the hopping term and the Hubbard interaction

$$T_{\beta}^{\alpha} = \sum_{\mathbf{n}} \sum_{j \in R} \left(\frac{1}{2} n_j (n_j - 1) - \mu n_j \right) U_{\mathbf{n}}^{\alpha} U_{\mathbf{n}}^{\beta} - t \sum_{\mathbf{n}} \sum_{\langle ij \rangle \in R} \left(\sqrt{n_i+1} \sqrt{n_j} U_{\{n_i+1, n_j-1\}}^{\alpha} U_{\mathbf{n}}^{\beta} + \sqrt{n_i} \sqrt{n_j+1} U_{\{n_i-1, n_j+1\}}^{\alpha} U_{\mathbf{n}}^{\beta} \right). \quad (15)$$

Bogoliubov matrix

The components of the mean field Hamiltonian of Eq. (10) in the Letter, $H^{(0)}$ and the matrices $A_{\mathbf{k}\alpha\beta}$ and $B_{\mathbf{k}\alpha\beta}$, are given by

$$\begin{aligned} H^{(0)} &= 2MW_{00}^{00}\sigma^4 + M(T_0^0 - \lambda)\sigma^2 \\ A_{\mathbf{k}\alpha\beta} &= (T_\beta^\alpha - \lambda\delta_{\alpha\beta}) + 2\sigma^2(W_{0\beta}^{\alpha 0}\gamma_{\mathbf{k}} + 2W_{\beta 0}^{\alpha 0}) + \frac{2}{M}\sum_{\mathbf{q}}\sum_{\alpha'\beta'}(W_{\beta'\beta}^{\alpha\alpha'}\Gamma_{\mathbf{k}\mathbf{q}} + 2W_{\beta\beta'}^{\alpha\alpha'})P_{\mathbf{q}\alpha'\beta'} \\ B_{\mathbf{k}\alpha\beta} &= \sigma^2W_{00}^{\alpha\beta}\gamma_{\mathbf{k}} + \frac{1}{M}\sum_{\mathbf{q}}\sum_{\alpha'\beta'}W_{\alpha'\beta'}^{\alpha\beta}\Gamma_{\mathbf{k}\mathbf{q}}K_{\mathbf{q}\alpha'\beta'} \end{aligned} \quad (16)$$

where we have defined $\Gamma_{\mathbf{k}\mathbf{q}} = \cos(Lk_x)\cos(Lq_x) + \cos(Lk_y)\cos(Lq_y)$. The density matrix $P_{\mathbf{q}\alpha\beta} = \langle b_{\mathbf{q}\alpha}^\dagger b_{\mathbf{q}\beta} \rangle = P_{\mathbf{q}\beta\alpha}^*$ is hermitian, and the pairing tensor $K_{\mathbf{q}\alpha\beta} = \langle b_{\mathbf{q}\alpha}^\dagger b_{-\mathbf{q}\beta}^\dagger \rangle = K_{-\mathbf{q}\beta\alpha}$ is symmetric. For the particular case of the Bose-Hubbard model, we assume that both of them are real.

Both matrices $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ depend on the density matrix and the pairing tensor, which were defined as expectation values in the Bogoliubov quasi-particle vacuum. Upon inversion of the Bogoliubov transformation, it is straightforward to show that

$$P_{\mathbf{k}\alpha\beta} = \sum_{\alpha'} Y_{\mathbf{k}\alpha\alpha'} Y_{\mathbf{k}\beta\alpha'}, \quad K_{\mathbf{k}\alpha\beta} = \sum_{\alpha'} Y_{\mathbf{k}\alpha\alpha'} X_{\mathbf{k}\beta\alpha'}. \quad (17)$$

Hartree-Bose matrix

Minimization of the free energy with respect to the condensed CB structure $U^{(0)}$ (see Eq. 18 in the letter), leads to the Hartree-Bose (HB) eigensystem:

$$\sum_{\mathbf{n}} h_{\mathbf{m},\mathbf{n}} U_{\mathbf{n}}^0 = \sum_{\mathbf{n}} (h_{\mathbf{m},\mathbf{n}}^{(0)} + h_{\mathbf{m},\mathbf{n}}^{(2)}) U_{\mathbf{n}}^0 = \lambda U_{\mathbf{m}}^0, \quad (18)$$

where we have separated the zeroth and second order contributions to the HB Hamiltonian.

The zeroth order has no contribution from fluctuating bosons, while the second order has quadratic contributions from fluctuating bosons

$$\langle H^{(0)} \rangle = 2MW_{00}^{00}\sigma^4 + M(T_0^0 - \lambda)\sigma^2, \quad (19)$$

$$\langle H^{(2)} \rangle = 2\sigma^2 \sum_{\mathbf{k}} \left(W_{00}^{\alpha\beta} \gamma_{\mathbf{k}} K_{\mathbf{k}\alpha\beta} + [W_{0\beta}^{\alpha 0} \gamma_{\mathbf{k}} + 2W_{\beta 0}^{\alpha 0}] P_{\mathbf{k}\alpha\beta} \right). \quad (20)$$

Making use of Eqs. (14) and (15) we first write explicitly the form of the tensors for the interaction and self-energy of the condensed CB entering in Eq. (19)

$$W_{00}^{00} = \frac{1}{2} \sum_{\langle i,j \rangle} \left(\sum_{\mathbf{n}} \sqrt{n_i + 1} U_{\{n_i+1\}}^0 U_{\mathbf{n}}^0 \right) \left(\sum_{\mathbf{n}'} \sqrt{n'_j + 1} U_{\{n'_j+1\}}^0 U_{\mathbf{n}'}^0 \right), \quad (21)$$

$$\begin{aligned} T_0^0 &= \sum_{\mathbf{n}} \sum_{j \in R} \left(\frac{1}{2} n_j (n_j - 1) - \mu n_j \right) U_{\mathbf{n}}^0 U_{\mathbf{n}}^0 \\ &\quad - t \sum_{\mathbf{n}} \sum_{\langle ij \rangle \in R} \left(\sqrt{n_i + 1} \sqrt{n_j} U_{\{n_i+1, n_j-1\}}^0 U_{\mathbf{n}}^0 + \sqrt{n_i} \sqrt{n_j + 1} U_{\{n_i-1, n_j+1\}}^0 U_{\mathbf{n}}^0 \right). \end{aligned} \quad (22)$$

The corresponding derivatives with respect to the condensate CB structure function are

$$\begin{aligned}
\frac{\partial}{\partial U_{\mathbf{m}}^0} W_{00}^{00} &= \frac{1}{2} \sum_{\langle i,j \rangle} \left(\sqrt{m_i+1} U_{\{m_i+1\}}^0 + \sqrt{m_i} U_{\{m_i-1\}}^0 \right) \left(\sum_{\mathbf{n}'} \sqrt{n'_j+1} U_{\{n'_j+1\}}^0 U_{\mathbf{n}'}^0 \right) \\
&\quad + \frac{1}{2} \sum_{\langle i,j \rangle} \left(\sum_{\mathbf{n}} \sqrt{n_i+1} U_{\{n_i+1\}}^0 U_{\mathbf{n}}^0 \right) \left(\sqrt{m_j+1} U_{\{m_j+1\}}^0 + \sqrt{m_j} U_{\{m_j-1\}}^0 \right) \\
&= \sum_{\langle i,j \rangle} \left(\sum_{\mathbf{n}} \sqrt{n_i+1} U_{\{n_i+1\}}^0 U_{\mathbf{n}}^0 \right) \left(\sqrt{m_j+1} U_{\{m_j+1\}}^0 + \sqrt{m_j} U_{\{m_j-1\}}^0 \right), \tag{23}
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial}{\partial U_{\mathbf{m}}^0} T_0^0 &= 2 \sum_{j \in R} \left(\frac{1}{2} m_j (m_j - 1) - \mu m_j \right) U_{\mathbf{n}}^0 \delta_{\mathbf{m}, \mathbf{n}} \\
&\quad - 2t \sum_{\langle ij \rangle \in R} \left(\sqrt{m_i} \sqrt{m_j+1} U_{\{m_i-1, m_j+1\}}^0 + \sqrt{m_i+1} \sqrt{m_j} U_{\{m_i+1, m_j-1\}}^0 \right). \tag{24}
\end{aligned}$$

Collecting terms, the zeroth order HB matrix is

$$\begin{aligned}
h_{\mathbf{m}, \mathbf{n}}^{(0)} &= \sum_{j \in R} \left(\frac{1}{2} m_j (m_j - 1) - \mu m_j \right) \delta_{\mathbf{m}, \mathbf{n}} \\
&\quad - t \sum_{\langle ij \rangle \in R} \left(\sqrt{m_i} \sqrt{m_j+1} \delta_{\mathbf{n}, \{m_i-1, m_j+1\}} + \sqrt{m_i+1} \sqrt{m_j} \delta_{\mathbf{n}, \{m_i+1, m_j-1\}} \right) \\
&\quad + \sigma^2 \sum_{\langle ij \rangle} \left[\left(\sum_{\mathbf{n}'} \sqrt{n'_i+1} U_{\{n'_i+1\}}^0 U_{\mathbf{n}'}^0 \right) \left(\sqrt{m_j+1} \delta_{\mathbf{n}, \{m_j+1\}} + \sqrt{m_j} \delta_{\mathbf{n}, \{m_j-1\}} \right) \right]. \tag{25}
\end{aligned}$$

Following a similar procedure, we obtain the second order contributions to the HB matrix (20). First we write explicitly the tensors for the interaction between two condensed bosons and two fluctuating bosons, and then their corresponding derivatives

$$W_{00}^{\alpha\beta} = \frac{1}{4} \sum_{\langle ij \rangle} \sum_{\mathbf{n}, \mathbf{n}'} \left(\sqrt{n_i+1} \sqrt{n'_j} U_{\{n_i+1\}}^\alpha U_{\{n'_j-1\}}^\beta U_{\mathbf{n}}^0 U_{\mathbf{n}'}^0 + \sqrt{n_i} \sqrt{n'_j+1} U_{\{n_i-1\}}^\alpha U_{\{n'_j+1\}}^\beta U_{\mathbf{n}}^0 U_{\mathbf{n}'}^0 \right), \tag{26}$$

$$\frac{\partial}{\partial U_{\mathbf{m}}^0} W_{00}^{\alpha\beta} = \frac{1}{4} \sum_{\langle ij \rangle} \sum_{\mathbf{n}} \left(\sqrt{n_i+1} \sqrt{m_j} U_{\{n_i+1\}}^\alpha U_{\{m_j-1\}}^\beta + \sqrt{n_i} \sqrt{m_j+1} U_{\{n_i-1\}}^\alpha U_{\{m_j+1\}}^\beta + [n \leftrightarrow m] \right) U_{\mathbf{n}}^0, \tag{27}$$

$$W_{0\beta}^{\alpha 0} = \frac{1}{4} \sum_{\langle ij \rangle} \sum_{\mathbf{n}, \mathbf{n}'} \left(\sqrt{n_i+1} \sqrt{n'_j+1} U_{\{n_i+1\}}^\alpha U_{\mathbf{n}}^0 U_{\mathbf{n}'}^0 U_{\{n'_j+1\}}^\beta + \sqrt{n_i} \sqrt{n'_j} U_{\{n_i-1\}}^\alpha U_{\mathbf{n}}^0 U_{\mathbf{n}'}^0 U_{\{n'_j-1\}}^\beta \right), \tag{28}$$

$$\frac{\partial}{\partial U_{\mathbf{m}}^0} W_{0\beta}^{\alpha 0} = \frac{1}{4} \sum_{\langle ij \rangle} \sum_{\mathbf{n}} \left(\sqrt{n_i+1} \sqrt{m_j+1} U_{\{n_i+1\}}^\alpha U_{\{m_j+1\}}^\beta + \sqrt{n_i} \sqrt{m_j} U_{\{n_i-1\}}^\alpha U_{\{m_j-1\}}^\beta + [n \leftrightarrow m] \right) U_{\mathbf{n}}^0, \tag{29}$$

$$W_{\beta 0}^{\alpha 0} = \frac{1}{4} \sum_{\langle ij \rangle} \sum_{\mathbf{n}} \left(\sqrt{n_i+1} \left[U_{\{n_i+1\}}^\alpha U_{\mathbf{n}}^\beta + U_{\mathbf{n}}^\alpha U_{\{n_i+1\}}^\beta \right] \right) \left(\sum_{\mathbf{n}'} \sqrt{n'_j+1} U_{\{n'_j+1\}}^0 U_{\mathbf{n}'}^0 \right), \tag{30}$$

$$\frac{\partial}{\partial U_{\mathbf{m}}^0} W_{\beta 0}^{\alpha 0} = \frac{1}{4} \sum_{\langle ij \rangle} \left(\sum_{\mathbf{n}'} \sqrt{n'_i+1} \left[U_{\{n'_i+1\}}^\alpha U_{\mathbf{n}'}^\beta + U_{\mathbf{n}'}^\alpha U_{\{n'_i+1\}}^\beta \right] \right) \left(\sqrt{m_j+1} U_{\{m_j+1\}}^0 + \sqrt{m_j} U_{\{m_j-1\}}^0 \right). \tag{31}$$

Making use of the W tensor derivatives, the second order term of the HB matrix is

$$\begin{aligned}
h_{\mathbf{m}, \mathbf{n}}^{(2)} &= \frac{1}{4M} \sum_{\langle ij \rangle} \left(\sqrt{n_i+1} \sqrt{m_j} U_{\{n_i+1\}}^\alpha U_{\{m_j-1\}}^\beta + \sqrt{n_i} \sqrt{m_j+1} U_{\{n_i-1\}}^\alpha U_{\{m_j+1\}}^\beta + [n \leftrightarrow m] \right) \left[\sum_{\mathbf{k}} \gamma_{\mathbf{k}} K_{\mathbf{k}\alpha\beta} \right] \\
&+ \frac{1}{4M} \sum_{\langle ij \rangle} \left(\sqrt{n_i+1} \sqrt{m_j+1} U_{\{n_i+1\}}^\alpha U_{\{m_j+1\}}^\beta + \sqrt{n_i} \sqrt{m_j} U_{\{n_i-1\}}^\alpha U_{\{m_j-1\}}^\beta + [n \leftrightarrow m] \right) \left[\sum_{\mathbf{k}} \gamma_{\mathbf{k}} P_{\mathbf{k}\alpha\beta} \right] \quad (32) \\
&+ \frac{1}{2M} \sum_{\langle ij \rangle} \left[\left(\sum_{\mathbf{n}'} \sqrt{n'_i+1} \left[U_{\{n'_i+1\}}^\alpha U_{\mathbf{n}'}^\beta + U_{\mathbf{n}'}^\alpha U_{\{n'_i+1\}}^\beta \right] \right) (\sqrt{m_j+1} \delta_{\mathbf{n}, \{m_j+1\}} + \sqrt{m_j} \delta_{\mathbf{n}, \{m_j-1\}}) \right] \left[\sum_{\mathbf{k}} P_{\mathbf{k}\alpha\beta} \right].
\end{aligned}$$